

Urea, (m-fluorophenyl)-
770-19-4 | DTXSID40227815

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.07

Global applicability domain: Inside

Local applicability domain index: 6.82e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Urea, 1-(p-fluorophenyl)-</div> <div>Measured: 1.04</div> <div>Predicted: 1.08</div>	<div>Image not found</div> <div>Urea, (m-fluorophenyl)-</div> <div>Measured: 1.29</div> <div>Predicted: 1.07</div>	<div>Image not found</div> <div>Urea, (3-methylphenyl)-</div> <div>Measured: 1.29</div> <div>Predicted: 1.08</div>
<div>Image not found</div> <div>(2-Fluorophenyl)urea</div> <div>Measured: 0.88</div> <div>Predicted: 8.30e-01</div>	<div>Image not found</div> <div>Benzylurea</div> <div>Measured: 0.73</div> <div>Predicted: 2.26e-01</div>	